SUPPLEMENTARY

Measuring Drug-Induced Changes in Metabolite Populations of Live Bacteria: Real Time Analysis by Raman Spectroscopy

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Figure S1. Raman difference spectrum of 1 μM H_2O_2 soaking into WT *K. pneumoniae* for 20 minutes.

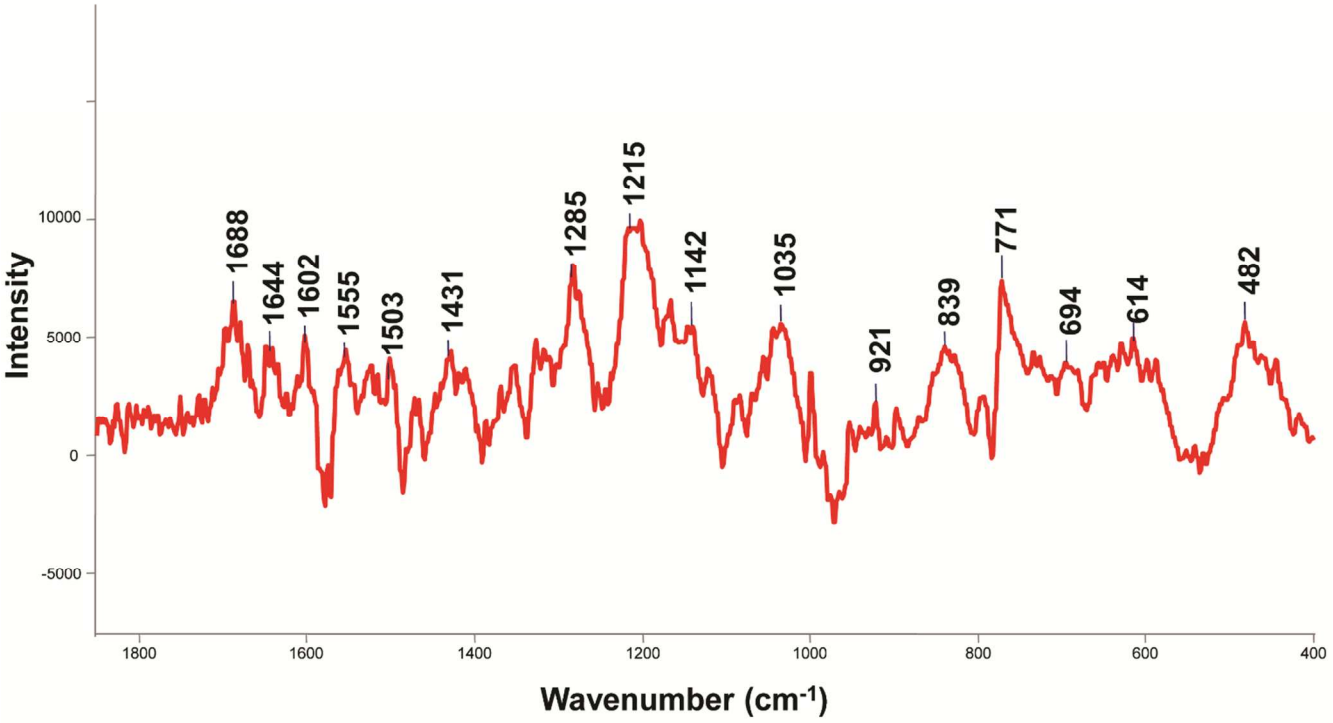

Figure S2. Raman spectrum of anhydrous sodium citrate.

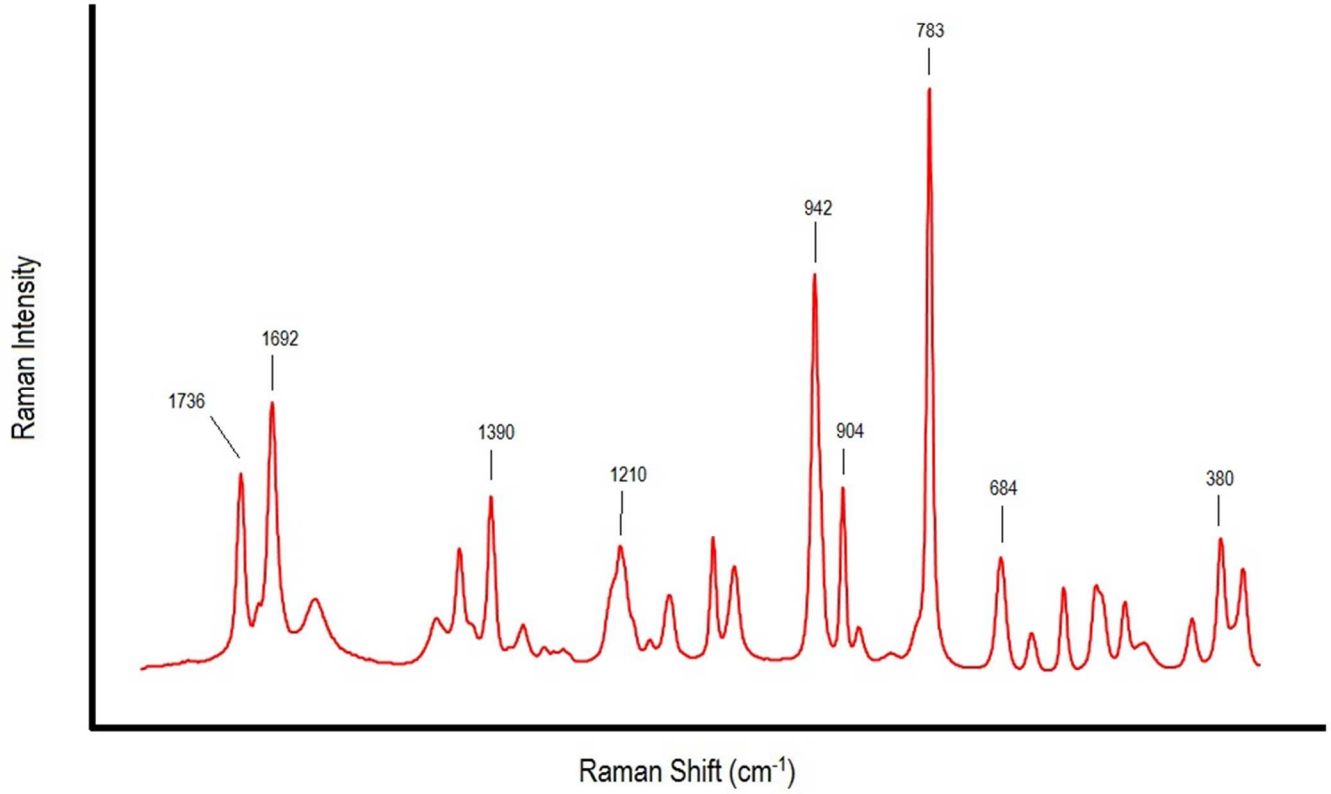

Table S1. Assignments for peaks seen in Figure 1, upper traces, unsubtracted spectra.

Wavenumber (cm^{-1})	Assignment
1668	amide I
1618	tyrosine ring
1606	phenylalanine ring
1572	guanine ring (major contributor), adenine ring (minor)
1475 (shoulder)	guanine ring
1449	CH_2 deformations
1350-1420	unresolved intensity due to carbohydrates
1332	adenine ring mode and CH2 deformation modes (non-aromatic residues), α-helices
1316	CH2 deformations (non-aromatic residues)
1241	amide III (disordered and β-sheet protein 2° structure)
1174	guanine ring
1142	thymine ring
1125	triphosphates from NTPs
1050-1130	phospholipids, carbohydrates, and PO_2^- in nucleic acids backbone
1031	phenylalanine ring
1003	phenylalanine ring
963	unassigned (possibly α-helices and/or carbohydrates)
806	RNA phosphodiester backbone (major contributor), DNA phosphodiester backbone (minor)
780	DNA phosphodiester backbone, RNA phosphodiester backbone (minor contributor), cytosine ring (minor contributor)
724	adenine ring
667	guanine ring
644	tyrosine ring
621	phenylalanine ring
577	guanine ring
475-600 (broad)	unassigned

Table S2. These are assignments to features in the Raman difference spectra in Figures 3-5.

Note	Wavenumber (cm-1)	Assignment
Nucleic Acids (all negative intensity):	1574	G ring (minor contribution from A ring)
	1482	G ring
	1340	A ring
	1127	Nucleotide triphosphate
	1100	-PO_2-, DNA and RNA backbone
	810	RNA backbone (minor contribution from DNA backbone)
	782	DNA backbone (minor contribution from RNA backbone)
	726	A ring
	670	G ring
	583	G ring ?
Proteins:	1000	Phenylalanine side chain
	1244-1250	Amide III disordered protein
	1650-6	Amide I α-helix